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# Density Functional Theory Approach to Nuclear Fission *

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The Skyrme nuclear energy density functional theory (DFT) is used to model neutron-induced fission in actinides. This paper focuses on the numerical implementation of the theory. In particular, it reports recent advances in DFT code development on leadership class computers, and presents a detailed analysis of the numerical accuracy of DFT solvers for near-scission calculations.

## 1. Introduction

In spite of successful applications in energy production and national security, relatively little is known about the fundamental mechanisms of the nuclear fission process. Even today, the most widely-used theories of fission rely on the macroscopic-microscopic approach to nuclear structure and semi-classical dynamics based on the Langevin equations. These methods are quite powerful but, in the long term, cannot be expected to yield the predictive power needed to understand the fission of very neutron-rich nuclei in the fission-recycling stage of the formation of elements, or to give enough accuracy for precise simulations of new generations of nuclear reactors.

Already in the 1980ies, promising attempts were made to understand fission in a microscopic framework based on the self-consistent nuclear mean-field theory with effective pseudo-potentials [1, 2]. At the time, the computing power was not sufficient for these approaches to compete with more empirical models, but these pioneer works yielded a lot of insight on the quantum mechanics of fission. In the recent years, the rapid development of leadership-class computers scaling to hundreds of thousands, and soon millions, of processing units has given us for the first time the computing power needed to successfully implement the full microscopic theory of fission. In parallel, novel forms of scientific collaborations gathering nuclear

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theorists, applied mathematicians and computer scientists have considerably improved our ability to utilize such large-scale machines [3].

The goal of this paper is to provide some tools to verify and validate DFT simulations of nuclear fission. In particular, we pay special attention to the problem of the numerical accuracy of DFT solvers at very large deformations. After a brief reminder on the theoretical framework, we recall some of the recent developments in DFT calculations on leadership class computers, then give a detailed analysis of truncation errors arising in DFT implementations using the one-center finite harmonic oscillator basis.

## 2. Theoretical Framework

The nucleus is described in the local density approximation at the Hartree-Fock Bogoliubov (HFB) approximation. The particle-hole channel is modeled by effective pseudo-potentials up to second-order derivatives in the density. In practice, this is equivalent to using zero-range effective interactions of the Skyrme type [4, 5]. The results presented below were thus obtained with the SkM* parameterization of the Skyrme interaction [6]. The particle-particle channel is characterized by a density-dependent contact interaction with mixed volume and surface character [7]. An energy cut-off of $E_{\text{cut}} = 60$ MeV is used to reduce the number of quasi- particles in the definition of the densities. The HFB equations are solved in a one-center harmonic oscillator basis.

In the DFT picture of nuclear fission, the HFB energy of the nucleus depends on an ensemble of collective variables $\boldsymbol{q} = (q_1, \ldots, q_N)$. These can be, for example, variables describing the nuclear shape, excitation or spin. In this work, we considered as collective variables the expectation value (on the HFB ground-state) of the multipole moments $\hat{Q}_{\lambda\mu}$. In practice, the axial $\hat{Q}_{20}$ and triaxial $\hat{Q}_{22}$, as well as the mass octupole $\hat{Q}_{30}$ and hexadecapole $\hat{Q}_{40}$ moments were considered. The collective space is thus four-dimensional.

In the actinide region, the part of the potential energy surface relevant to nuclear fission spans a rather large range in deformations. The axial quadrupole moments runs typically from $\sim 30$ b in the ground-state to nearly 600 b at scission for symmetric fission; the octupole moment from 0 to about 70 b$^{3/2}$ for very asymmetric fission (cluster radioactivity, see [8, 9]); the hexadecapole moment from nearly $\sim 3$ b$^2$ near the ground-state to typically more than $\sim 350$ b$^2$ for symmetric fission. Assuming for sake of simplicity a uniform sampling of each degree of freedom, and a 1 b$^{\lambda/2}$ mesh size, the size of the collective space is more than 1.4 millions points, only for the axial collective variables. Adding triaxiality multiplies this estimate by another 2 orders of magnitude.

## 3. Large-Scale Potential Energy Surfaces

In this section, we present the performance of our DFT solver, and provide a detailed analysis of convergence properties of our Skyrme HFB calculations in the case of $^{240}$Pu.

### 3.1. DFT Solvers on Leadership Class Computers

All calculations were performed with the DFT solvers HFBTHO [10] and HFODD [11]. Both codes solve the HFB equations in the harmonic oscillator (HO) basis. The program HFBTHO assumes axial and time-reversal symmetry, while HFODD is fully symmetry-unrestricted. The two programs have been benchmarked against one another and agree within a few eV for an axial configuration [10] .
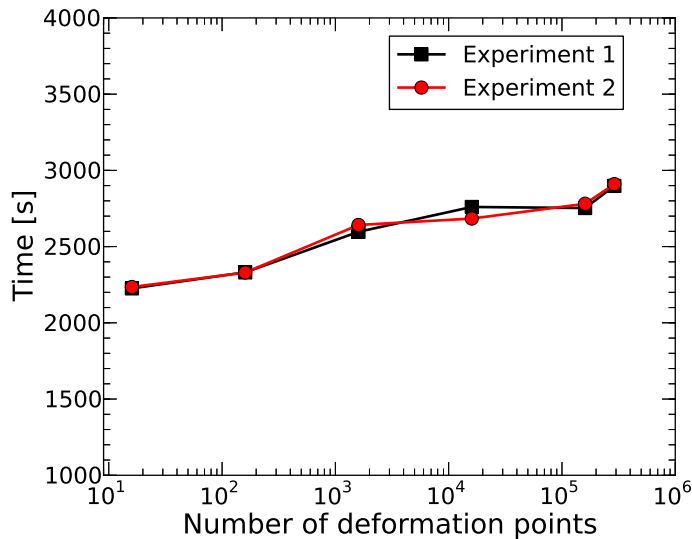


Fig. 1. Performance of the DFT solver HFODD on the Titan supercomputer at the Oak Ridge Leadership Computing Facility in Oak Ridge. Each experiment measures the time of performing six full HFB iterations. The term 'deformation point' refers to a set of constraints on multipole moments, i.e. a point in the collective space.

Owing to the block-diagonal structure of the HFB matrix induced by axial symmetry, the typical runtime of HFBTHO is of the order of the minute (depending on the type of nucleus, size of the basis and 'difficulty' of converging the HFB iterations). By contrast, it is of the order of several

hours for HFODD. In practice, HFBTHO is used as pre-conditioner for HFODD: for any given point $\boldsymbol{q}$ in the collective space, the HFB iterations are first solved with HFBTHO, and the densities at convergence are used to initialize HFODD. If the point of the collective space is axial, no additional iterations are therefore needed.

Clearly, the very large size of the collective space together with the current runtime of the DFT solvers requires using today's most powerful supercomputers. A lot of effort was, therefore, devoted to porting our codes to leadership class computers, and ensuring that good scaling with the number of processing units could be achieved. From a computational point of view, mapping the nuclear collective space in DFT is a naturally parallel problem. The code HFODD has, therefore, a hybrid MPI/OpenMP programming model, where points in the collective space are distributed across the MPI grid, and on-node multi-threading enables to take advantage of highly optimized linear algebra libraries. Figure 1 shows the performance of HFODD on the Titan supercomputer at the Oak Ridge Leadership Computing Facility. In this experiment, up to 300,000 processors were used in parallel. The slight degradation of the computing time is due to the original input/output backend, which has not been optimized and taxes the operating system at large scale.

### 3.2. Numerical Accuracy

Modeling nuclear fission requires to explore regions of the collective space with extreme deformations. The finite size of the HO basis may thus lead to a significant dependence of the results on the basis parameters. In our calculations, we only considered axially-deformed bases, characterized by a quadrupole deformation $\beta$ and an oscillator frequency $\omega_0$. The maximum number of shells is denoted by $N_{\mathrm{max}}$ and the maximum number of states by $N_{\mathrm{states}}$. In the case of a full spherical HO basis, the two are related through the well-known relation $N_{\mathrm{states}} = (N_{\mathrm{max}} + 1)(N_{\mathrm{max}} + 2)(N_{\mathrm{max}} + 3)/6$. This relation is not valid anymore for a deformed basis. In practice, we introduce two cut-offs, one on the number of shells and another on the number of states. Note that the cut-off on the number of states is only the practical consequence of using a symmetry-unrestricted solver, for which the size of the matrices involved goes approximately as $2N_{\mathrm{max}}^3$. By contrast, the block structure induced by the built-in axial symmetry in HFBTHO would enable to consider all full shells up to $N_{\mathrm{max}}$.

Basis dependence of the calculations thus comes from 4 parameters (i) the maximum number of shells $N_{\mathrm{max}}$, (ii) the maximum number of states $N_{\mathrm{states}}$, (iii) the oscillator frequency $\omega$ and (iii) the basis deformation $\beta_2$. In principle, at every point $\boldsymbol{q}$ in the collective space, we should seek the

HFB solution that is the minimum in this 4-dimensional parameter space. Clearly, such a strategy is not sustainable even on today's largest computers. Instead, one is bound to estimate truncation errors by exploring the parameter space locally, and extracting asymptotic expressions.
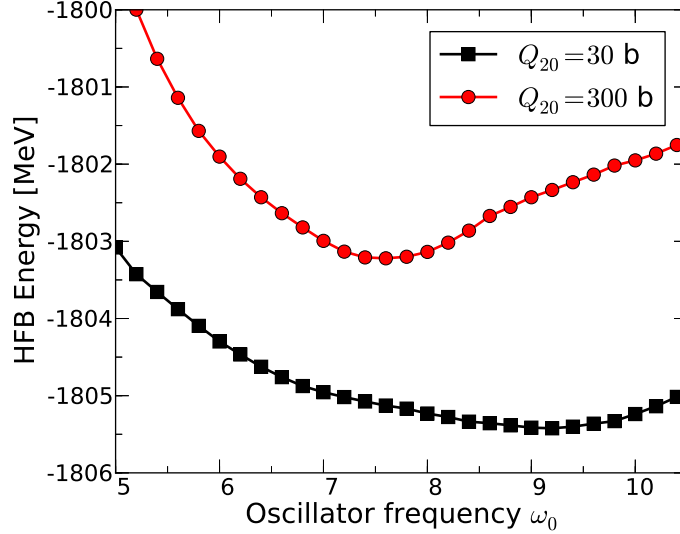


Fig. 2. (color online) Convergence of the HFB energy as function of the oscillator frequency $\omega_0$, for two configurations characterized by $q_{20} = 30$ b (black squares) and $q_{20} = 300$ b and $q_{40} = 120$ b$^2$ (red circles). The deformation $\beta$ is adjusted according to the formula (2).

As a first example, we show in figure 2 the dependence of the HFB energy on the spherical-equivalent frequency of the harmonic oscillator $\omega_0$, that is the frequency such that $\omega_0^3 = \omega_x \omega_y \omega_z$. The deformation of the basis is fixed at each point according to the formula (2). Two typical points in the collective space are considered, one near the ground-state with deformation $\langle \hat{Q}_{20} \rangle = 30$ b, one way past the second barrier on the descent to scission at $\langle \hat{Q}_{20} \rangle = 300$ b. We note that the dependence on $\omega_0$ is more marked at large deformations, and that the optimal frequency shifts toward smaller values as the deformation increases, which is consistent with the need to then include basis states with a larger spatial extension. Importantly, it is possible to extend this analysis and extract an empirical fit $\omega_0(Q_{20})$ giving the optimal basis frequency as function of the quadrupole moment of the collective point. In our tests, we found that the expression

$$\omega_0 = \begin{cases} 0.1 \times q_{20} e^{-0.02 q_{20}} + 6.5 \text{MeV if } |q_{20}| \leq 30 \text{b} \\ 8.14 \text{MeV if } |q_{20}| > 30 \text{b} \end{cases} \tag{1}$$

gives a reasonably accurate fit of the frequency as function of the quadrupole moment.
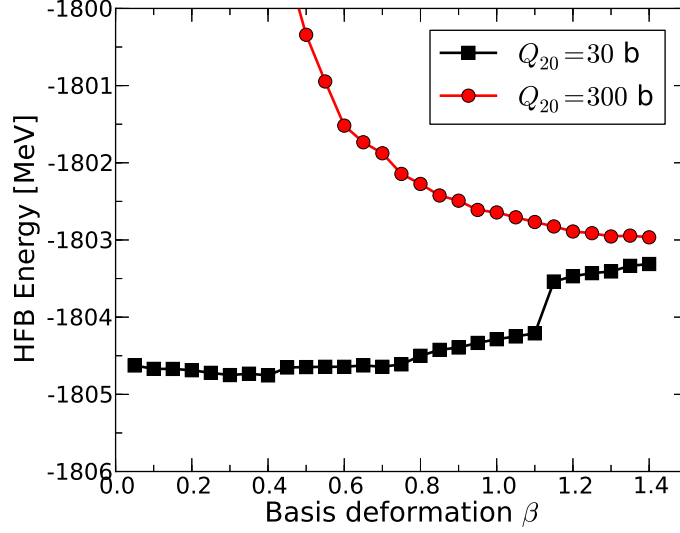


Fig. 3. (color online) Convergence of the HFB energy as function of the basis deformation $\beta$. The oscillator frequency is adjusted according to the formula (1). For the second configuration, an additional constraint on $\hat{Q}_{60}$ to $q_{60} = 150$ b$^3$ was added.

The dependence of the HFB energy on the deformation of the basis, for a fixed $N_{\text{max}}$ and basis deformation, is illustrated in figure 3. Not surprisingly, the minimum is always obtained for basis deformation that are 'close' to the requested value of the axial quadrupole moment. Note that the dependence on deformation is rather marked. However, as for the oscillator frequency, it is *a priori* possible to obtain a fit $\beta(Q_{20})$ such that the optimal basis deformation is chosen at point in the collective space. Our tests showed that the simple formula

$$\beta = 0.05\sqrt{q_{20}} \tag{2}$$

provides a reasonable expression that remains applicable up to the largest values of $\hat{Q}_{20}$.

Last but not least, we show in figure 4 the error induced by the truncation of the number of states. Contrary to the previous two parameters of the HO basis, this truncation is imposed by memory limitations, and can not really be mitigated: for a given value of $N_{\text{max}}$, the optimal number of states is always given by $N_{\text{states}} = (N_{\text{max}} + 1)(N_{\text{max}} + 2)(N_{\text{max}} + 3)/6$, a number that can grow very large for large $N_{\text{max}}$ For example, at $N_{\text{max}} = 30$,
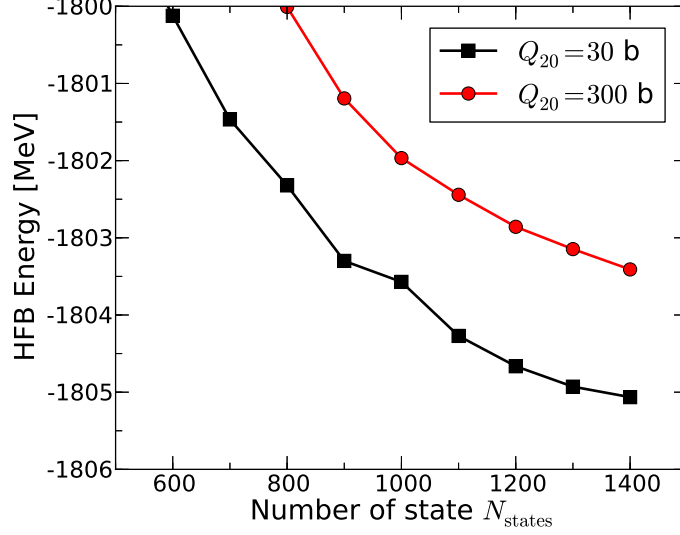
Fig. 4. (color online) Convergence of the HFB energy as function of the number of states $N_{\text{states}}$.

we have $N_{\text{states}} = 5456$. Taking into account the spin degree of freedom, the total number of basis states is more than 10,000, which implies that the size of the HFB matrix exceeds $20{,}000 \times 20{,}000$. At this time, it is not possible to handle in a reasonable time frame iterative processes involving dense, complex matrices in double precision of that size. As can be seen from figure 4, restricting $N_{\text{states}}$ to manageable values around $N_{\text{states}} \approx 1000\text{-}1200$ may easily lead to 2 to 3 MeV errors beyond the second fission barrier.

To finish this section, we would like to emphasize two important consequences of basis truncation effects:

- At constant truncation, the error increases with deformation, albeit not necessarily linearly. This is bound to have a very significant impact for, e.g., calculations of barrier penetrability, since the numerical precision is not the same at the entry and exit points, and errors of the order of the MeV can lead to orders of magnitude uncertainties on fission lifetimes;

- Truncations magnify the impact of discontinuities in the potential energy landscape. In practice, calculations with very different basis characteristics initialized with similar density/wave-functions could converge to two very different points of the multi-dimensional PES. This effect is the reason why, in the lower panel of figure 3, an addi-

tional constraint on $\hat{Q}_{60}$ had to be added: without it the calculation did not converge to the same point in the collective space at small and large basis deformations.

## 4. Conclusions

The nuclear energy density functional theory is currently the only viable option to achieve a microscopic description of nuclear fission. On-going development of leadership class computing facilities all over the world offer a unique opportunity to finally develop the nuclear DFT at very high precision. In this work, we have discussed some of the numerical uncertainties associated with implementations of DFT in the one-center harmonic oscillator basis. They clearly point to the need of developing bases that are better adapted to the extreme elongations characterizing the region near scission.

## 5. Acknowledgments

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